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Optimization of sourness and flavor in orange-flavored gummy candies using a simplex-lattice mixture design implemented with R

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Optimización de la acidez y del aroma en caramelos de goma con sabor a naranja utilizando un diseño de mezclas simplex-lattice implementado con R

Abstract

Acidulants are crucial for enhancing and balancing the flavor profiles of confectionery products, such as gummy candies, ensuring an optimal sensory experience. This study aimed to develop an R script using the simplex-lattice mixture design to optimize the sourness and flavor levels and the combined response of these attributes for orange-flavored gummy candies, demonstrating its application in improving the sensory qualities of confectionery products. The gummy candies were prepared according to previous research, incorporating citric, malic, and fumaric acids based on the experimental design. The R scripts were provided and uploaded to the GitLab platform for download and analysis (https://gitlab.com/FoodChem-DataSci-Lab/orange-flavored-gummy-candies). The effects of these acids on sourness and flavor were assessed using a 5-point hedonic scale by 30 trained judges. The data were analyzed with R, resulting in mathematical models for the acids' individual effects, interactions, and combined responses. Effect (Piepel direction) and contour plots were generated as well. The optimal mixture was determined to be 4.95 g of citric acid, 4.65 g of malic acid, and 5.40 g of fumaric acid, achieving an optimal combined response value of 107.14. In conclusion, balancing these three acids is critical to optimizing sourness and flavor levels in orange-flavored gummy candies. This study provided a valuable methodology for formulating confectionery products with enhanced sensory profiles. It demonstrated the capability of R to address complex problems in both the confectionery industry and academia, emphasizing its importance as an analytical tool for developing products with improved sensory characteristics.

Keywords: Gummy candies, acidulants, Simplex-lattice mixture design, hedonic scale, R programming

Resumen

Los acidulantes son cruciales para mejorar y equilibrar los perfiles de sabor de los productos

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de confitería, como los caramelos de goma, asegurando una experiencia sensorial óptima. Este estudio tuvo como objetivo desarrollar un script en R utilizando el diseño de mezclas simplex-lattice para optimizar los niveles de acidez y aroma y la respuesta combinada de estos atributos para caramelos de goma con sabor a naranja, demostrando su aplicación para mejorar las cualidades sensoriales de los productos de confitería. Los caramelos de goma se prepararon según investigaciones previas, incorporando ácidos cítrico, málico y fumárico con base en el diseño experimental. Los scripts en R se proporcionaron y cargaron en la plataforma GitLab para su descarga y análisis (https://gitlab.com/FoodChem-DataSci-Lab/orange-flavored-gummy-candies). Treinta jueces capacitados evaluaron los efectos de estos ácidos sobre la acidez y el aroma utilizando una escala hedónica de 5 puntos. Los datos se analizaron con R, lo que dio como resultado modelos matemáticos para los efectos individuales, las interacciones y las respuestas combinadas de los ácidos. También se generaron gráficos de efectos (dirección de Piepel) y gráficos de contornos. Se determinó que la mezcla óptima era 4.95 g de ácido cítrico, 4.65 g de ácido málico y 5.40 g de ácido fumárico, logrando un valor de respuesta combinado óptimo de 107.14. En conclusión, equilibrar estos tres ácidos es fundamental para optimizar los niveles de acidez y aroma en los caramelos de goma con sabor a naranja. Este estudio proporcionó una metodología valiosa para formular productos de confitería con perfiles sensoriales mejorados. Demostró la capacidad de R para abordar problemas complejos tanto en la industria de la confitería como en el mundo académico, enfatizando su importancia como herramienta analítica para desarrollar productos con características sensoriales mejoradas.

Palabras clave: Caramelos de goma, acidulantes, diseño de mezclas simplex-lattice, escala hedónica, programación en R

INTRODUCTION

Gummy candies are primarily made from saturated solutions of refined sucrose and corn syrups (glucose 42 DE). However, sucrose can also be replaced with polyols such as isomalt or erythritol [1]. These ingredients are mixed and heated to a cooking temperature between 106 and 120°C, with pre-hydrated gelatin added, although other hydrocolloids can also be used. Finally, food additives such as colorants, flavorings, and acidulants are incorporated into the mixture [1,2,3].

The flavoring agents and the acidulants are critical for enhancing flavor perception in these products. The importance of flavor in consumer acceptance is fundamental in the food industry. A food's palatability, determined by its taste and other sensory characteristics, drives consumer preferences and choices, significantly influencing a product's acceptability and market success [4,5,6]. The addition of acidulants, such as citric, malic, and fumaric acids, in citrus-flavored gummy candies plays a vital role in improving the flavor profile by adding sourness, freshness, and balance to the citrus taste, creating a pleasant and satisfying sensory experience for consumers [7,8,9].

One of the main challenges in the confectionery industry is product formulation and reformulation. Statistical methods such as the simplex-lattice mixture design have addressed this issue. This approach systematically and efficiently explores the interaction between multiple ingredients in varying proportions, which is critical for achieving

optimal sensory and nutritional properties, maximizing efficiency, and reducing the need for numerous tests and trials [10,11,12].

The scientific community has long debated the merits of R and Python for experiment design, with both languages offering distinct advantages. R is powerful in statistical analysis and experimental design, especially for complex tasks like mixture experiments. Its robustness in handling these designs has been well-documented, making it a popular choice in research and industries like food, pharmaceuticals, and chemicals. Several studies in the literature highlight the effectiveness of these R packages in practical applications [13]. The R package 'mixexp' is handy for generating mixture designs, which can be challenging to implement in other languages, including Python [14]. For example, in a study, the use of 'mixexp' was reported to optimize the formulation of a food product, achieving results that were not easily replicable using other software platforms [10]. This package optimizes responses based on component proportions, offering specialized functions for designing mixtures under linear and nonlinear constraints—an essential feature in many experimental contexts [10,14,15]. While Python is praised for its ease of use and intuitive syntax, it does not match R's capabilities in complex experimental designs, particularly for mixtures. Although Python has packages like Salmon and Pymix that offer similar functionality, they do not yet reach the depth and specialization of R's tools [16]. Furthermore, R's extensive and well-documented statistical packages make it invaluable in academic research, where precision and detailed analysis are critical [17].

When comparing R and Python to proprietary software like Design Expert, several advantages of open-source programming languages stand out. While Design Expert provides advanced design capabilities, it is costly and offers limited flexibility for customization beyond its graphical interface. In contrast, R and Python are free, removing the financial barrier of expensive licenses and providing greater flexibility and customization due to their open-source nature [18]. This accessibility allows researchers to utilize powerful analytical tools without the burden of high costs. R and Python's flexibility also enables users to tailor their code to specific requirements, which is critical for conducting complex experiments. In academic settings, using R and Python also fosters collaboration and knowledge-sharing. As open-source software, they allow researchers to share scripts and methodologies, promoting reproducibility and transparency in research [19,20]. This contrasts with proprietary software, where access to source code and underlying methodologies is often restricted, potentially hindering the verification of results and replication of studies [21].

Therefore, in educational environments, R and Python offer extensive tutorials, documentation, and community support, facilitating the learning and implementation of advanced data analysis techniques [22]. This is particularly valuable in academia, where continuous learning and access to educational resources are essential for researchers' professional development. As open-source and free, R is widely accessible across academic, industrial, and research settings, helping to bridge the digital divide by providing advanced tools without the burden of high costs.

Based on the above, the objective of this study was to develop R scripts using the simplex-lattice mixture design to optimize the sourness and flavor levels and the combined response of these attributes for orange-flavored gummy candies. The aim was to provide

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step-by-step explained scripts applied to a practical case, demonstrating how these tools can enhance the sensory properties of products in the confectionery industry.

MATERIALS AND METHODS

Preparation of gummy candies

The gummy candies were prepared following a formulation and process provided for academic purposes by a confectionery company in Mineral de la Reforma, Hidalgo, Mexico. Due to the nature of the project, citing the details of the process or the quantities of ingredients and food additives used was not permitted, except in the final stage related to the addition of acidifying agents. At this stage, for a mixture of water, refined sucrose, and corn syrup previously cooked at a specific temperature and combined with hydrated gelatin wholly dissolved, a liquor prepared with artificial orange flavoring, orange artificial coloring, water, and 15 g of an acid blend (citric, fumaric, and malic acids) was added, adjusted according to the simplex-lattice mixture design shown in Table 1. Finally, the mixture of all ingredients and food additives was homogenized and dosed into drop-shaped silicone molds. The gummy candies were left to solidify and rest for a specified time, then de-molded, coated with refined sugar, and left to rest for an additional period. Finally, they were stored in airtight glass containers until used for sensory analysis.

TABLE 1. Experimental design and mass fraction of the three acids used in the formulation of orange-flavored gummy candies according to the simplex-lattice mixture design.

	Uncoded values (fractions of the acids)			Coded values (g)		
Index	x1	x2	x3	Citric acid	Malic acid	Fumaric acid
M1	1	0	0	15	0	0
M2	0.5	0.5	0	7.5	7.5	0
M3	0	1	0	0	15	0
M4	0.5	0	0.5	7.5	0	7.5
M5	0	0.5	0.5	0	7.5	7.5
M6	0	0	1	0	0	15
M7	0.75	0.25	0	11.25	3.75	0
M8	0.75	0	0.25	11.25	0	3.75
M9	0.5	0.25	0.25	7.5	3.75	3.75
M10	0.25	0.75	0	3.75	11.25	0
M11	0.25	0.5	0.25	3.75	7.5	3.75
M12	0.25	0.25	0.5	3.75	3.75	7.5
M13	0	0.75	0.25	0	11.25	3.75
M14	0.25	0	0.75	3.75	0	11.25
M15	0	0.25	0.75	0	3.75	11.25

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Sensorial analysis

The sensory analysis was conducted as described in previous research, with modifications [23,24,25]. A group of 30 trained panelists, all students of the Bachelor's Degree in Food Chemistry at the Universidad Autónoma del Estado de Hidalgo, Mexico, conducted the sensory evaluation to identify the analyzed attributes (sourness and flavor). The samples were individually presented to evaluators on cardboard plates labeled with three-digit characters. The panelists provided scores from 1 to 5 for each attribute analyzed as follows: Sourness: 1 = very slightly intense, 2 = slightly intense, 3 = adequate, 4 = intense, and 5 = very intense. Flavor: 1 = dislike, 2 = neither like nor dislike, 3 = like slightly, 4 = like moderately, and 5 = like very much.

The number of scores for each point on the hedonic scale was multiplied by the corresponding coefficient, and the cumulative sum for each evaluated formulation was calculated to use the value as a response variable. Equation 1 represents this:

$$\mathbf{y} = \sum_{i=1}^{5} n_i c_i \tag{1}$$

where $\mathbf{y}$ is the response value (sourness, flavor, or combined level), n_i is the number of scores for point i on the scale, and c_i is the coefficient for point i on the scale.

R scripts

All scripts used to produce the results of the analyses presented in this document were implemented using the R programming language (v.4.1.2, "Bird Hippie") and the integrated development environment RStudio® (v.2024.04.2) on a computer running the elementary OS 7.1 Horus operating system (based on Ubuntu 22.04.3 LTS, Linux 6.5.0-44-generic). The libraries used included 'mixexp', 'Ternary', 'viridisLite', 'PlotTools', 'stats', and 'dplyr'. All scripts are also provided as executable R files with their respective documentation, datasets, and model summaries. Everything has been uploaded to GitLab so that interested parties can access them for analysis and implementation (https://gitlab.com/FoodChem-DataSci-Lab/orange-flavored-gummy-candies).

Simplex-Lattice mixture design configuration

First, an R file named "simplex_lattice_design.R" was created, and the script used to define and configure the mixture design was developed. This design was established according to the procedures described in previous research [26,27,28]. In the script, the mixexp library was used to set up a simplex-lattice mixture design with three factors: citric acid (x_1), malic acid (x_2), and fumaric acid (x_3), as well as two additional levels at zero using the SLD function **(simplex_lattice_desing_1 <- SLD(fac = 3, lev = 2))**. Subsequently, the design was enriched with interior points using the Fillv function **(simplex_lattice_design_2 <- Fillv(3, simplex_lattice_design_1))**, ensuring complete coverage of the experimental space, as this configuration generated 15 different mixtures [14,15,29].

The factors were coded by multiplying the values by 15 to obtain the amounts of the acids in grams **(simplex_lattice_desing_2$citric_acid <- 15 * simplex_lattice_desing_2$x1**, etc.). To visualize the combinations, the 'TernaryPlot' library was used

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to set up the ternary plot, and the AddToTernary function was used to add the points and experiment numbers, thereby generating an index of experiments within the plot **(AddToTernary(graphics::points, data_points, pch = 21, cex = 4, bg = "white"))**. This plot can be seen in Figure 1. Finally, the design was exported to a CSV file **(write.csv(simplex_lattice_design_2, file = "simplex_lattice_design_ORANGE.csv", row.names = FALSE))**, facilitating the subsequent analysis of experimental data and the optimization of the gummy candies' sourness and flavor levels. The resulting experiment matrix can be seen in Table 1.

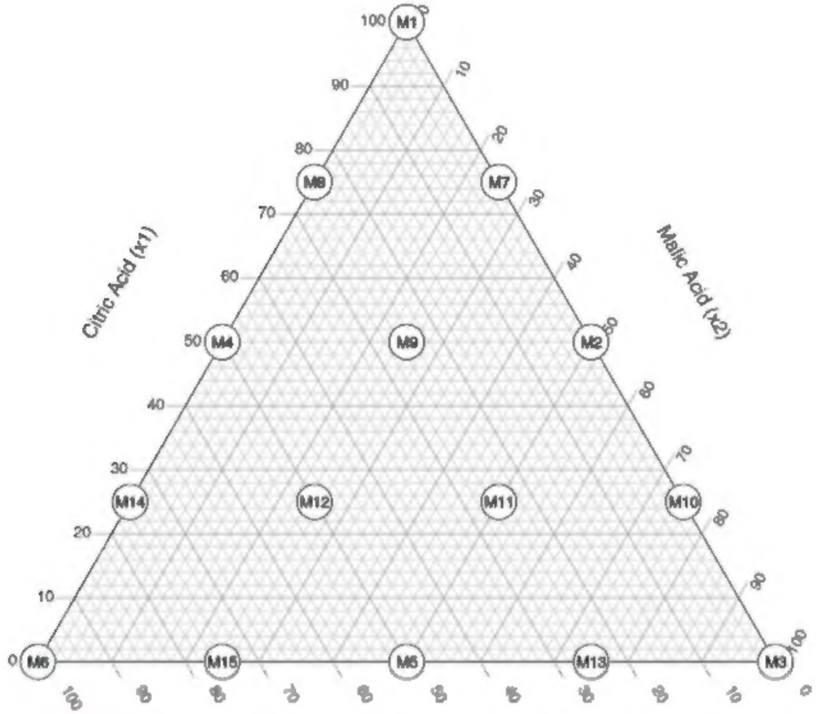

FIGURE 1: Arrangement of mixture points using the simplex-lattice design method in a ternary plot.

The selection of the simplex-lattice mixture design was driven by its specific suitability for experiments where the response variables are functions of the proportions of the components in a mixture rather than their absolute quantities. The elements' proportions (factors) are involved in mixture designs, and the mix's total amount is usually fixed. This means that the quantity of each component is proportional to the total mixture, and unlike in factorial designs, the proportions of the elements cannot vary independently since they are constrained by the requirement that their sum must be constant (1 or 100%). This interdependency is a critical characteristic that distinguishes mixture designs from other approaches like Central Composite Design or Box-Behnken Design, where factors can vary independently. The analysis in mixture designs is conducted through

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a response surface, which allows for the identification of the optimal mixture [30,31]. This approach is particularly appropriate for optimizing formulations in food science, where the balance of ingredients directly influences the product's sensory attributes. Previous studies have demonstrated the effectiveness of this design in similar contexts, supporting its application in this work [24,28,29,30,31]. The advantages of using a simplex-lattice mixture design include a comprehensive exploration of the experimental space with fewer trials and the ability to capture complex interactions between components [32], thereby providing a robust framework for optimizing the sensory properties of the orange-flavored gummy candies.

ANALYSIS OF RESULTS

R scripts were created to perform the statistical analysis of the results. Below is a general explanation of the script used to analyze the influence of the factors on the sourness level; however, the script for flavor level analysis was similar. Both scripts have been uploaded to GitLab as executable R files in the project directory. Initially, necessary libraries such as 'mixexp', 'Ternary', 'viridisLite', 'PlotTools', and 'stats' were loaded. The experimental results dataset was imported using **read.csv("sourness.csv").**

The optimization model was constructed using the linear regression function **lm**, which considered the main effects and interactions of citric acid (**x1**), malic acid (**x2**), and fumaric acid (**x3**) on the sourness level (**y**) **(sourness_model <- lm(y ~ x1 + x2 + x3 + x1:x2 + x1:x3 + x2:x3 + x1:x2:x3 -1, data = dataset))** [28,33,34]. This is in accordance with Equation 2:

$$y = \beta_1 x_1 + \beta_2 x_2 + \beta_3 x_3 + \beta_{12} x_1 x_2 + \beta_{13} x_1 x_3 + \beta_{23} x_2 x_3 + \beta_{123} x_1 x_2 x_3 \quad (2)$$

where **y** is the estimated response (sourness, flavor, or combined level), and β_1, β_2, β_3, β_{12}, β_{13}, β_{23}, and β_{123} are constant coefficients for each linear and non-linear interaction term.

The model summary was saved to a text file using capture for documentation purposes. **output(summary(sourness_model), file = "summary_model_sourness.txt")**.

To visualize the effects of the mixture components, an effect plot (Piepel direction) was generated and saved as a PNG file at 300 DPI **(EffPlot(des = dataset, mod = 2, dir = 1))**. The 'TernaryPlot' library was used to display the response surface of the model in a ternary plot format, defining a function to contour the response surface **(FunctionToContour <- function(a, b, c) { predict(sourness_model, newdata = data.frame(x1 = a, x2 = b, x3 = c)) })**. Contour lines and experiment data points, labeled with experiment numbers, were added to the plot **(AddToTernary(graphics::points, data_points, pch = 21, cex = 4, bg = "white"))**. A continuous legend for the color scale was also included to indicate the intensity of the response.

Finally, the optimal combination of the mixture was determined using a function that predicted sourness levels based on the model coefficients **(coefficients <- coef(sourness_model))**. This function, **sourness_level**, calculated the predicted

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sourness for given levels of the three acids, incorporating interactions among them. A grid of possible mixtures was created, and the optimal mixture with the highest predicted sourness was identified **(result <- predict_best_mixture())**. The results, including the optimal values for **x1**, **x2**, and **x3**, along with the corresponding sourness level, were saved to a text file **(writeLines(results,"optimal_sourness_level_results.txt"))**. This analysis facilitated the determination of the ideal formulation to achieve the desired sourness in the orange-flavored gummy candies.

Combined model

The file "combined_model.R" was created to develop a combined model integrating the sourness and flavor levels in orange-flavored gummy candies. The goal was to determine the optimal combination of citric acid (**x1**), malic acid (**x2**), and fumaric acid (**x3**) to maximize both responses. The following describes each stage of the process, including the code used and an explanation of its purpose and functionality. This script has been uploaded to GitLab as an executable R file in the project directory.

Initially, necessary libraries such as 'mixexp', 'Ternary', 'viridisLite', 'PlotTools', 'stats', and 'dplyr' were loaded. The datasets containing experimental results for sourness and flavor were imported using **read.csv("sourness.csv")** and **read.csv("flavor.csv")**, respectively.

Separate linear regression models were developed for sourness and flavor levels using the **lm** function, considering main effects and interactions among acids **(sourness_model <- ...** and **flavor_model <- ...)**, excluding the intercept [28,33]. A combined dataset was created by merging the sourness and flavor datasets and calculating a combined response variable **(combined_dataset <- ...)**. The combined response variable **y_combined** is calculated as the average of **y_sourness** and **y_flavor**, giving equal weight to both sensory properties. This combined measure provided a holistic view of the product's sensory profile.

The combined model was then developed using the **lm** function **(combined_model_lm <- lm(y_combined ~ x1 + x2 + x3 + x1:x2 + x1:x3 + x2:x3 + x1:x2:x3 -1, data = combined_dataset))**, excluding the intercept, and the summary was saved to a text file ("summary_combined_model.txt"). A function, **combined_model**, was defined to predict responses based on the combined model **(combined_model <- function(a, b, c) ...)**. It uses three arguments, **a**, **b**, and **c**, representing the proportions of acids to create a new data frame. Then, the **predict** function was used to generate predictions from the **combined_model_lm** model with this new data set, returning the predicted result [26].

For visualization, the **EffPlot** function was used to create an effects plot, saved as a PNG file. A ternary plot was generated to illustrate the response surface, including contour lines representing the combined response **(TernaryPlot(alab = "Citric acid (x1)", ...)** [14,15]. The optimal combination of **x1**, **x2**, and **x3**, yielding the highest combined response, was identified using a grid search approach **(predict_best_combined_mixture())**, with results saved to a text file ("optimal_combined_level_results.txt"). The optimal point was also highlighted in the ternary plot **(AddToTernary(graphics::points, matrix(unlist(optimal_values), ncol = 3), pch = 19, col = "red", cex = 2))**. This analysis comprehensively evaluated the optimal mixture to balance sourness and flavor in the orange-flavored gummy candies.

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RESULTS AND DISCUSSION

Sourness level model

The sourness level model demonstrated high accuracy, as indicated by the Multiple R-squared value of 0.9926 and an adjusted R-squared of 0.9926 (Table 2). These values suggested that the model explained approximately 99.26% of the variance in the sourness response, highlighting the model's predictive solid capability. The coefficients for the primary factors, citric acid (x_1), malic acid (x_2), and fumaric acid (x_3), were all statistically significant, with p-values below 0.05. The coefficient estimates were 80.759 for x_1, 89.474 for x_2, and 90.545 for x_3, indicating that these acids contributed significantly to the sourness level. However, the interaction terms, including x_1:x_2, x_1:x_3, x_2:x_3 and x_1:x_2:x_3, were not statistically significant, suggesting that the combined effects of these acids did not significantly influence the sourness beyond their individual contributions. The model's residual standard error was 11.140, reflecting the average deviation of the observed data points from the fitted model, and the F-statistic of 153.4 indicated a highly significant model overall, with a p-value of 6.919×10^{-8}.

Table 2. Model coefficients and statistical summary for sourness level, flavor level, and combined levels models.

Model	Coefficients	Standard Error	R^2	R^2-adjusted	Residual Standard Error	p-value	F-statistic
Sourness level	x_1: 80.759 x_2: 89.474 x_3: 90.545 x_1:x_2: 42.836 x_1:x_3: 26.550 x_2:x_3: 40.836 x_1:x_2:x_3: 40.296	x_1: 9.905 x_2: 9.905 x_3: 9.905 x_1:x_2: 46.054 x_1:x_3: 46.054 x_2:x_3: 46.054 x_1:x_2:x_3: 286.911	0.9926	0.9926	11.140	6.919×10^{-8}	153.4
Flavor level	x_1: 96.045 x_2: 113.545 x_3: 107.688 x_1:x_2: 3.122 x_1:x_3: 43.693 x_2:x_3: −48.593 x_1:x_2:x_3: 216.296	x_1: 9.702 x_2: 9.702 x_3: 9.702 x_1:x_2: 45.113 x_1:x_3: 45.113 x_2:x_3: 45.113 x_1:x_2:x_3: 281.047	0.9945	0.9945	10.910	2.119×10^{-8}	206.7
Combined level	x_1: 88.402 x_2: 101.509 x_3: 99.116 x_1:x_2: 22.979 x_1:x_3: 35.122 x_2:x_3: −3.878 x_1:x_2:x_3: 128.296	x_1: 6.112 x_2: 6.112 x_3: 6.112 x_1:x_2: 28.417 x_1:x_3: 28.417 x_2:x_3: 28.417 x_1:x_2:x_3: 177.036	0.9975	0.9975	6.872	8.845×10^{-10}	459.5

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Flavor level model

The flavor model also exhibited strong performance, with a Multiple R-squared value of 0.9945 and an adjusted R-squared of 0.9945, indicating that 99.45% of the variance in the flavor response was explained by the model. The coefficient estimates for citric acid (x_1), malic acid (x_2), and fumaric acid (x_3) were 96.045, 113.545, and 107.688, respectively. These values demonstrated that malic acid had the highest influence on flavor, followed by fumaric and citric acids. The standard errors for these coefficients were relatively small, suggesting precise estimates. Unlike the sourness model, the flavor model showed a significant interaction term for x_1:x_3, with a coefficient estimate of 43.693, indicating a notable combined effect of citric and fumaric acids on flavor. The model's residual standard error was 10.910, slightly lower than the sourness model's, indicating a better fit. The F-statistic was 206.7, with a p-value of 2.119×10^{-8}, confirming the overall statistical significance of the model.

Combined sourness and flavor level model

The combined model, which integrated sourness and flavor responses, achieved the highest accuracy among the three models. It had a Multiple R-squared value of 0.9975 and an adjusted R-squared of 0.9975, suggesting that the model explained 99.75% of the variance in the combined response. The coefficient estimates for citric acid (x_1), malic acid (x_2), and fumaric acid (x_3) were 88.402, 101.509, and 99.116, respectively, indicating that malic acid was the dominant contributor to the combined response, followed closely by fumaric and citric acids. The interaction term x_1:x_2 was also notable, with a coefficient estimate of 128.296, suggesting a significant three-way interaction effect on the combined response. The residual standard error of 6.872 was the lowest among the models, indicating an exact fit. The F-statistic was 459.5, with a p-value of 8.845×10^{-10}, underscoring the solid overall significance of the combined model.

Effect (Piepel direction) and Contour plots

In analyzing the sourness level, the effects of citric acid (x_1), malic acid (x_2), and fumaric acid (x_3) on orange-flavored gummy candies were evaluated. The effect plot (Piepel direction) showed the predicted sourness response as a function of deviation from the centroid for each component (Figure 2a) [35,36]. Citric acid (x_1) had the most significant effect, peaking above 100, while malic acid (x_2) and fumaric acid (x_3) had smaller, similar effects. Each curve reached local maxima, indicating optimal concentration points for each acid. The contour plot in Figure 2a, a ternary diagram, depicted the response surface for sourness based on the proportions of the acids. Lighter areas indicated higher sourness, with the highest level (around 100) in the central yellow area [37], suggesting synergy between the acids. Sourness decreased as one acid became dominant, especially at the vertices. Optimal combinations for high sourness were near the center, with roughly equal proportions of the three acids, indicating that a balanced mixture optimized sourness in the orange-flavored gummy candies.

The optimal combination of acids to maximize the sourness level was determined with the R script, using the fitted model and the **predict_best_mixture** function, as described in the Materials and Methods sections. The analysis revealed that the best mixture consisted of 2.7 g of citric acid (x_1), 6.45 g of malic acid (x_2), and 5.85 g of fumaric acid (x_3), achieving

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a predicted sourness level of 101.57. These results confirm that a balanced combination of the three acids is adequate for optimizing the sourness in the orange-flavored gummy candies, providing valuable guidance for the final product formulation.

Concerning flavor level analysis, the effect plot (Figure 2b) showed that the citric acid (x_1) had a significant quadratic effect, peaking and decreasing. Malic acid (x_2) decreased flavor liking with deviation while fumaric acid (x_3) showed a slight decrease followed by an increase with less impact than x_1 and x_2 [36,38]. Citric acid had the most pronounced effect on flavor liking followed by malic and fumaric acid. The ternary contour plot (Figure 2b) depicted the response surface for the acid combinations. Contour lines indicated flavor level, with blue for lower and yellow for higher flavor level. The highest liking areas (yellow) were centered around specific acid combinations, showing an optimal blend. The best combinations included moderate citric acid and lower malic and fumaric acids. This plot showed how the acid combinations affected flavor level, helping identify the optimal proportions for maximizing this sensory attribute.

The analysis with the R script computed the best combination of the three acids, yielding the following proportions: 6 g of citric acid (x_1), 2.4 g of malic acid (x_2), and 6.6 g of fumaric acid (x_3). This combination resulted in a maximum flavor level of 114.53. This result revealed that higher proportions of citric acid and fumaric acid significantly contribute to flavor liking, while a smaller amount of malic acid is beneficial. The graphical analysis supports this conclusion, showing that citric acid has a pronounced positive effect on flavor perception, while malic acid has a less favorable impact. The optimal interaction between these acids highlights the importance of balancing their proportions to achieve the best sensory profile.

Finally, the combined analysis with R integrated sourness and flavor level responses. The effect plot (Figure 2c) showed how citric acid (x_1), malic acid (x_2), and fumaric acid (x_3) influenced the combined response. Malic acid (x_2) had the highest predicted response followed by fumaric acid (x_3) and citric acid (x_1), with each acid showing a peak followed by a decline. The contour plot (Figure 2c) depicted the combined response surface with the optimal point near the center (a red point). The best combination was 4.95 g of citric acid, 4.65 g of malic acid, and 5.4 g of fumaric acid, achieving a combined optimal response of 107.14. This indicates that balancing the three acids optimizes both sourness and flavor levels. The slightly higher proportion of fumaric acid suggests its vital role in enhancing the combined response.

All three models demonstrated high accuracy and statistical significance, with the combined model providing the most comprehensive explanation of the data variance. The inclusion of interaction terms in the combined model underscored the importance of considering the joint effects of the acids on the sensory characteristics of orange-flavored gummy candies. This analysis using the R programming language offered practical guidance for adjusting gummy formulations to ensure that consumers optimally perceive both sourness and flavor. Future research should include confirmatory experiments, as this study primarily aimed to demonstrate the optimization of a confectionery product with R. There are limited examples in scientific journals that show step-by-step R scripts, which could greatly benefit researchers, students, food developers, and others interested in the topic.

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Finally, while no studies have directly compared the performance of Python, R, and Design Expert in the context of simplex lattice design, both Python and R are recognized as powerful tools for data analysis, each with distinct advantages. Design Expert, by contrast, offers a more user-friendly option for those seeking to perform experimental designs without programming. Future research should prioritize direct comparisons to clarify the strengths and limitations of each tool in this specific context.

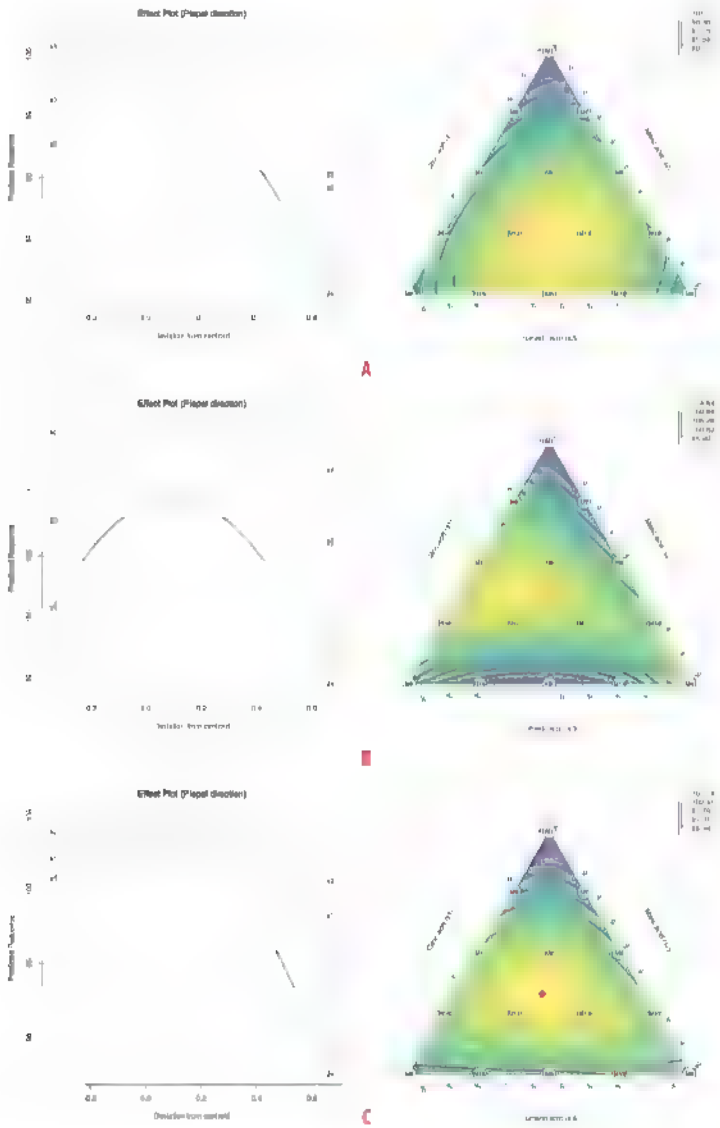

FIGURE 2: Influence of citric (x1), malic (x2), and fumaric (x3) acids on sourness level (a), flavor level (b), and combined level of sourness and flavor (c) in orange-flavored gummy candies. Effect (Piepel direction) and Contour Plots.

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CONCLUSIONS

This study optimized the flavor profile of orange-flavored gummy candies using a simplex-lattice mixture design implemented in the R programming language. The key findings indicated that the optimal combination of acids to maximize flavor liking was 6 g of citric acid, 2.4 g of malic acid, and 6.6 g of fumaric acid, achieving a maximum liking score of 114.53. The developed regression models allowed for the evaluation of the individual effects of each acid and their binary and ternary interactions without considering an intercept. The assessment of the coefficients and the statistical significance of each term determined the specific influence of each acid and their combinations on sourness and flavor levels, providing a valuable tool for optimizing formulations and improving the final product quality. These results offer guidance for gummy manufacturers, food technologists, and others interested in the topic, enabling them to adjust formulations to maximize consumer satisfaction.

The research also emphasized the importance of using open-source software like R to optimize confectionery product formulations. As open-source and free software, R allowed for complex and detailed analyses in an accessible and efficient manner, facilitating the evaluation of the individual and combined effects of acids on the gummy flavor profile. This accessibility could contribute to reducing research costs and promote democratizing access to advanced analytical tools, fostering innovations in the food industry and food science research.

Prospects of this research include applying the developed methodology to other flavors and types of confectionery products to validate and extend the findings. Additionally, it is recommended that other acidulants and their impact on the sensory profile of products be explored, as well as the implementation of emerging technologies in food formulation and processing to further improve product quality and acceptance. The research can also extend to shelf-life and stability studies, ensuring optimized formulations maintain their sensory properties over time.

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CREDIT AUTHORSHIP CONTRIBUTION STATEMENT

Lizbeth Chávez-Reyes: Writing – original draft, Investigation. **Laura García-Curiel:** Methodology, Software. **Jesús Guadalupe Pérez-Flores:** Writing – original draft, Software, Conceptualization. **Emmanuel Pérez-Escalante:** Writing – review & editing. **Elizabeth Contreras-López:** Writing – review & editing. **Lizbeth Anahí Portillo-Torres:** Validation. **Luis Guillermo González-Olivares:** Validation. **Carlos Ángel-Jijón:** Validation.

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